Proper Dirac Quantization of Free Particle on D-Dimensional Sphere

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We show that an unambiguous and correct quantization of the second-class constrained system of a free particle on a sphere in D dimensions is possible only by converting the constraints to abelian gauge constraints, which are of first class in Dirac's classification scheme. The energy spectrum is equal to that of a pure Laplace-Beltrami operator with no additional constant arising from the curvature of the sphere. A quantization of Dirac's modified Poisson brackets for second-class constraints is also possible and unique, but must be rejected since the resulting energy spectrum is physically incorrect.

1. Quantization of a free point particle in curved space is a long-standing and controversial problem in quantum mechanics. Dirac has emphasized that canonical quantization rules are consistent only in a Cartesian reference frame [1]. Attempts to generalize these rules to curved space run into the notorious *operator-ordering problem* of momentum and coordinates, making the Hamiltonian operator non-unique. Podolsky [3] avoided this problem by *postulating* that the Laplacian in the free Schrödinger operator $H = -\hbar^2 \Delta/2$ should be replaced by the Laplace-Beltrami operator $\Delta_{\text{LB}} = g^{-1/2}\partial_\mu g^{1/2}g^{\mu\nu}\partial_\nu$, where $\partial_\mu = \partial/\partial q^\mu$ are the partial derivatives with respect to the D-dimensional curved-space coordinates, and g is the determinant of the metric $g_{\mu\nu}(q)$. This postulate has generally been accepted as being correct since it yields, for a D-dimensional sphere of radius R embedded in a $D+1$-dimensional Cartesian space with coordinates x^i, an energy $\hat{L}_a^2/2R^2$. Here $\hat{L}_a = -i\hat{p}_i(L_a)_{ij}x_j$ with $\hat{p}_i = -i\hbar\partial/\partial x_i$ are the unique quantum-mechanical differential operator representation of the $D(D+1)/2$ generators L_a of the rotation group $\text{SO}(D+1)$ in flat space. If we take a to label the index pairs ij with $i \leq j$, then L_a are the matrices $(L_{ij})_{kl} = i(\delta_{ik}\delta_{jl} - \delta_{ik}\delta_{jl})$, whose nonzero commutation rules are

$$[L_{ij}, L_{ik}] = -iL_{jk} \quad \text{(no sum over } i\text{)}. \tag{1}$$

The canonical commutation rules $[\hat{p}_i, \hat{x}_j] = -i\hbar\delta_{ij}$ transfer the Lie algebra (1) to the operators $\hat{L}_{ij}/\hbar$. The square of the total angular momentum $\hat{L}_a^2$ is the Casimir operator of the orthogonal group SO(D+1), with the eigenvalues $l(l + D - 1)$, $l = 0, 1, 2, \ldots$ [4]. Thus, by quantizing classical angular momentum rather than canonical variables (i.e., by putting hats on L's rather than on p's) operator-ordering problems are avoided, making this energy spectrum the most plausible one [5].

Doubts on the correctness of this spectrum have been raised by DeWitt [6] in his first attempt to quantize the system by a straightforward generalization of Feynman's time-sliced path integral to curvilinear coordinates. He found an extra energy proportional to the Riemannian scalar curvature $\bar{R}$ of in the Schrödinger operator:

$$H = -\frac{\hbar^2}{2}\Delta_{\text{LB}} + \alpha\hbar^2\bar{R}, \tag{2}$$

with a proportionality constant $\alpha = 1/24$. Various successors have presented modifications of DeWitt's procedure leading to other proportionality factors $\alpha = 1/12$ [7] and $\alpha = 1/8$ [8].

For the above sphere, the extra term produces an extra constant energy equal to $\alpha\hbar^2 D(D-1)/R^2$ which would contradict the previous results. At fist sight, this contradiction seems to be rather irrelevant. Common experiments are only capable of detecting *energy differences*, in which this constant drops out. Cosmology, however, is sensitive to an additive constant, which would change the gravitational energy of interstellar rotating two-atomic gases. Apart from such somewhat esoteric applications, a correct quantization of this simplest non-Euclidean system is certainly of fundamental theoretical interest.

It is therefore important to find physical systems for which the $\bar{R}$-term is not a constant, so that it can distort the energy spectrum of the Schrödinger operator (2). Such a system has recently been found, although in a somewhat indirect way. When solving the path integral of the hydrogen atom, a two-step nonholonomic mapping is needed which passes through an intermediate non-Euclidean space [9,10]. The existence of an extra $\bar{R}$-term in (2) would modify significantly the known level spacings in the hydrogen spectrum. Thus experiment eliminates an extra curvature scalar, in agreement with Podolsky and with the quantization of angular momentum. The successful procedure was generalized into a simple *nonholonomic mapping principle*, which allows to map classical and quantum-mechanical laws in flat space into correct laws in curved space [9–11].

The absence of an $\bar{R}$-term in (2) is therefore a crucial test for any quantum theory in curved spaces. It is the purpose of this note to show that this absence can be established for a sphere also within the operator approach to quantum mechanics, after suitably preparing the description for an application of Dirac's theory of constrained systems.

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This application is, however, not straight-forward. A D-dimensional sphere is most simply described by embedding it into a $D + 1$ -dimensional Cartesian x-space via a constraint $x^2 - R^2 = 0$. Within Dirac's classification scheme [2], such a constraint is of second class. We shall demonstrate that Dirac's quantization rules for such systems produce wrong energy levels. A correct quantization becomes possible only by making use of a recently developed conversion [13] of second-class constraints to first-class constraints, which instead of configuration space restrict the quantum-mechanical *Hilbert space* [2]. This conversion requires an extension of the phase space of the initial Cartesian system to a larger auxiliary Cartesian phase space, where the correct quantization is known. The operators representing the first-class constraints are generators of gauge transformations, and the physical states are all found by going into the gauge invariant subspace of the Hilbert space.

Constraints associated with gauge symmetry have first been mastered in quantum electrodynamics (Coulomb's law), and are now a standard tool in the quantization of gauge theories [12].

2. We begin by quantizing the system with the help of Dirac's theory for second-class constraints. A free point particle with a Hamiltonian $H = p^2/2$ moving in a flat Euclidean $D + 1$-dimensional is restricted to the surface of a D-dimensional sphere by the primary constraint in configuration space [2]

$$\varphi_1 = x^2 - R^2 = 0 . \tag{3}$$

The dynamical consistency condition $\dot{\varphi}_1 = \{H, \varphi_1\} = 0$ leads to an additional secondary constraint in phase space

$$\varphi_2 = (x, p) = 0 . \tag{4}$$

It expresses the fact that a motion on a sphere has no radial component. Although the canonical variables are Cartesian, the canonical quantization is not applicable, since the constraints (3), (4) cannot be enforced for the associated operators — the conditions $\hat{\varphi}_1 = \hat{\varphi}_2 = 0$ would be in conflict with the commutation relation $[\hat{\varphi}_1, \hat{\varphi}_2] = 2i\hbar\hat{x}^2 = 2i\hbar R^2 \neq 0$. To resolve this difficulty, Dirac replaced the Poisson symplectic structure $\{x_i, p_j\} = \delta_{ij}$ by the so-called *Dirac brackets*

$$\{A, B\}_D = \{A, B\} - \{A, \varphi_a\}[\Delta^{-1}]^{ab}\{\varphi_b, B\} , \tag{5}$$

where Δ_{ab} is a matrix $\Delta_{ab} = \{\varphi_a, \varphi_b\}$ formed from all primary and secondary constraints $\varphi_a = 0$. This matrix is assumed to be non-degenerate, a defining property of second-class constraints [2]). The Dirac brackets provide us with an antisymmetric operation which is distributive and associative, i.e., which satisfies Leibnitz rule and Jacobi identity, thus forming a symplectic structure which is as good as Poisson's.

The removal of the inconsistency is ensured by the automatic property

$$\{A, \varphi_a\}_D = 0 , \quad \text{for any } A \text{ and } \varphi_a . \tag{6}$$

Hamiltonian equations of motion generated by the Dirac bracket $\dot{A} = \{A, H\}_D$ coincide with those generated by the original Poisson bracket $\{ , \}$ on the surface of constraints $\varphi_a = 0$. Thus, Dirac brackets produce classically the same equations of motion as Poisson brackets. Quantization proceeds by the replacement $\{ , \}_D \to -i[,]/\hbar$. The property (6) allows us to replace the constraints by operator equations $\hat{\varphi}_a = 0$ without the earlier contradictions. Moreover, since the constraint operators $\hat{\varphi}_a$ commute with any other operator, they can be given any c-number value, for instance zero. For the surface of the sphere, the quantized Dirac brackets (5) read

$$[\hat{x}_i, \hat{x}_j] = 0 ; \tag{7}$$

$$[\hat{x}_j, \hat{p}_k] = i\hbar \left(\delta_{jk} - \frac{\hat{x}_j\hat{x}_k}{\hat{x}^2} \right) ; \tag{8}$$

$$[\hat{p}_j, \hat{p}_k] = i\hbar\frac{1}{\hat{x}^2}(\hat{p}_j\hat{x}_k - \hat{p}_k\hat{x}_j) . \tag{9}$$

The operator ordering problem occurring in the right-hand side of (9) is uniquely resolved under the condition that the algebra (7)–(9) satisfies the Jacobi identity. The operator $\hat{x}^2$ commutes with all canonical operators and is therefore a c-number, which can be set equal R^2.

To find the spectrum of the Hamiltonian $\hat{H} = \hat{p}^2/2$, we make use of the identity

$$\delta_{ij} = -\frac{(L_a\hat{x})_i(L_a\hat{x})_j}{\hat{x}^2} + \frac{\hat{x}_i\hat{x}_j}{\hat{x}^2} . \tag{10}$$

Inserting this into $\hat{p}^2 = \hat{p}_i\delta_{ij}\hat{p}_j$, we obtain the Hamiltonian

$$\hat{H} = \frac{1}{2R^2}\hat{L}_a^2 + \frac{1}{2}\hat{p}_r^\dagger\hat{p}_r , \tag{11}$$

where $\hat{L}_a = -i\hat{p}_i(L_a)_{ij}\hat{x}_j$ as before and $\hat{p}_r = (\hat{x}, \hat{p})/R$ is a radial momentum operator. Note that the operator (11) is determined without operator-ordering ambiguities. The identity (10) can equally well be inserted to the left and the right of the momentum operators $\hat{p}_i\hat{p}_j$, with a unique result.

The radial operator $\hat{p}_r$ commutes with all canonical operators and is therefore some complex number c. It has necessarily an imaginary part, due to the obvious relation $\hat{p}_r - \hat{p}_r^\dagger = i\hbar D/R$ implied by (8). Thus we may decompose $\hat{p}_r = c = i\hbar D/2R + c_r$, where c_r is an arbitrary real number. The constant c_r is determined by expressing $\hat{p}_r$ in terms of the operator of the second constraint (4). The ordering of $\hat{p}$ and $\hat{x}$ in it is undetermined, so that $\hat{\varphi}_2$ may be written as $(\hat{p}_r + \hat{p}_r)/2 + i\hbar\gamma$ with an arbitrary imaginary part γ. Inserting the above constant for $\hat{p}_r$ and setting $\hat{\varphi}_2$ equal to zero is solved uniquely by $\gamma = 0$ and $c_r = 0$.

It is now easy to find the spectrum of the first term in the Hamiltonian operator (11). The modified canonical rules (7)–(9) transfer the Lie algebra (1) to the operators $\hat{L}_a = -i\hat{p}L_a\hat{x}$ in just the same way as ordinary canonical

commutation rules, so that the energy levels of angular momentum l are

$$E_l = \frac{\hbar^2}{2R^2} l(l + D - 1) + \frac{1}{8R^2}\hbar^2 D^2 . \tag{12}$$

The additional constant energy has a different D-dependence than the $\bar{R}$-term proposed by DeWitt and others [7,8]. In particular, it is nonzero even for a particle on a circle ($D = 2$), where nobody ever expected such a term.

Thus the modified symplectic structure proposed by Dirac, although esthetically appealing and yielding a unique result for a particle on the surface of a sphere, must be rejected on physical grounds as contradicting the established quantization via angular momentum operators and nonholonomic mapping principle.

3. In second-class constrained systems, not every phase space variable can be made an operator. Dirac's new symplectic structure (5) represented by (7)–(9) accounts for this fact via its degeneracy in the embedding phase space. This permits the canonical variables of fluctuations transverse to the manifold on which the particle moves to remain c-numbers. There is, however, a defect in Dirac's procedure: Although physical excitations of the transverse degree of freedom are eliminated, the system maintains a memory of the forbidden motion by a nonzero c-number valued transverse energy $\hat{p}_r^\dagger\hat{p}_r/2$. From the physical point of view, the existence of such a memory must be rejected. After all, the embedding space is only an artifact for the introduction Euclidean canonical commutation rules. It does not belong to the manifold where the particle moves. An alternative approach must therefore be found where a memory of the embedding space is absent.

Such an alternative is offered by gauge theories. In these, equations of motion exhibit symmetries which are local in time with the consequence that the dynamics of some degrees of freedom is not specified by the equations of motion. Such local symmetries are gauge symmetries, and the undetermined degrees of freedom correspond to pure gauge configurations. Upon quantization, non-physical degrees of freedom are removed by restricting the Hilbert space to a physical subspace formed by gauge invariant states.

Thus, rather than restricting the particle motion to the surface of a sphere via constraints as above, we consider a free motion in a Cartesian coordinate system, and impose the condition that the physical states in Hilbert space are invariant under arbitrary time-dependent rescalings of the radial size of the system. The transverse momentum $\hat{p}_r$ can be made a generator of gauge transformations, and we may require $\hat{p}_r^\dagger\hat{p}_r$ to be zero for physical states.

To achieve this goal, we invoke the method of abelian conversion that allows one to transform a second-class constrained system into an abelian gauge theory [13]. Dynamics of physical (gauge invariant) degrees of freedom in the effective abelian theory is the same as dynamics of physical degrees of freedom in the original second-class constrained system. In general, the abelian conversion proceeds as follows. Given a set of second-class constraints φ_a ($a = 1, 2, \ldots, 2M$), one extends the original phase space by extra independent canonical variables Q_α, P_α ($\alpha = 1, 2, \ldots, M$). The extended phase space is equipped with the canonical symplectic structure $\{Q_\alpha, P_\beta\} = \delta_{\alpha\beta}$ and $\{x_i, p_j\} = \delta_{ij}$ (all other brackets are zero). With the help of abelian conversion, quantum dynamics on a manifold can be formulated independently of the parametrization of the manifold [14].

An equivalent set of abelian first-class constraints $\sigma_a = 0$ is constructed in such a way that it satisfies

$$\{\sigma_a, \sigma_b\} = 0. \tag{13}$$

This amounts to solving first-order differential equations with the boundary condition $\sigma_a(x, p, P = 0, Q = 0) = \varphi_a(x, p)$. Given the new constraints $\sigma_a = 0$, the original system Hamiltonian $H(x, p)$ is converted into a Hamiltonian on the extended phase space $\bar{H}(x, p, P, Q)$ by solving the equation

$$\{\bar{H}, \sigma_a\} = 0 \tag{14}$$

with the boundary condition $\bar{H}(x, p, Q = 0, P = 0) = H(x, p)$. The extrema of the associated extended action $S^{\text{ext}} = \int dt(p_i\dot{x}_i + P_\alpha\dot{Q}_\alpha - \bar{H} - \lambda_a\sigma_a)$ determine equations of motion in the extended phase space. These depend on $2M$ arbitrary functions of time $\lambda_a(t)$ as a manifestation of the gauge freedom. There exists a choice for $\lambda_a(t)$ such that the auxiliary phase space variables $P_\alpha(t)$ and $Q_\alpha(t)$ vanish at all times, whereas $p_i(t)$ and $x_i(t)$ solve the original equations of motion of the second-class constrained system [13].

Applying this procedure to our particular second-class constraints (3) and (4) yields

$$\sigma_1 = \varphi_1 + P , \quad \sigma_2 = \varphi_2 + 2x^2 Q , \tag{15}$$

while the extended Hamiltonian assumes the form

$$\bar{H} = \frac{1}{2}\left(\frac{\sigma_2^2}{\sigma_1 + R^2} + \frac{L_a^2}{\sigma_1 + R^2}\right) , \tag{16}$$

where $L_a = -ipL_a x$ are the classical components of the angular momentum (for $a = ij$, $L_a = x_i p_j - x_j p_i$). The extended phase space variables p, x, P, Q are Cartesian and satisfy the standard Poisson bracket relations. They can be turned into hermitian operators in the usual way by the replacement $\{\ ,\ \} \rightarrow -i[\ ,\ ]/\hbar$

Physical states are invariant with respect to transformations generated by $\sigma_{1,2}$: $x \rightarrow e^{-\xi_2}x$ and $Q \rightarrow Q - \xi_1$, where $\xi_{1,2}$ are parameters of the gauge transformations [14]. The first is an arbitrary time-dependent rescaling of the size of the system, which is geometrically equivalent to the initial restriction of the motion to the surface of the sphere, while the second implies that the auxiliary degree

of freedom is a pure gauge. The first-class constraints restrict the physical Hilbert space to the gauge-invariant sector by the Dirac conditions [2]

$$\hat{\sigma}_{1,2}\Psi_{\text{phys}} = 0 \ . \tag{17}$$

The general solution has the form $\Psi_{\text{phys}} = f(Q, x^2)\Psi(\Omega)$, where $f(x, Q)$ is some fixed function, whereas $\Psi(\Omega)$ are wave functions on the D-sphere. In the physical Hilbert space, we can set $\sigma_{1,2}$ to zero in the Hamilton operator (16). Thus we find the energy values

$$E_l = \frac{\hbar^2}{2R^2}l(l + D - 1) \ , \tag{18}$$

rather than (12). There is no additional constant energy, in agreement with [3,5,9].

This result is obtained without ordering problems. Although ordering ambiguities are not absent altogether, they do not affect the final result since they occur only in the quantization of the gauge generator σ_2, where they modify only the explicit form of the physically irrelevant function $f(x^2, Q)$, but not the physical Hilbert space described by the wave function $\Psi(\Omega)$, nor the spectrum (18). In fact, in the simple system at hand the ordering ambiguities in $\hat{\sigma}_2$ produce only a multiplicative renormalization of the physical states Ψ_{phys}.

4. The above quantization of a particle on a sphere via abelian conversion is of course applicable to arbitrary homogeneous spaces. But what about arbitrary manifolds? When attempting a straight-forward generalization we run once more into operator-ordering problems for the extended Hamiltonian (16), and these require a new strategy. The quantum Hamiltonian $\hat{H} = \hat{p}^2/2$ has no ordering ambiguity and is again adopted as a starting point. Let $n(x)$ be a unit vector normal to the manifold in the embedding space (if this space has a dimension higher than $D + 1$, more normal vectors are needed to specify transverse directions). The condition $\hat{p}_n\Psi_{\text{phys}} = (n(\hat{x}), \hat{p})\Psi_{\text{phys}} = 0$ removes the transverse motion and offers itself as a generator of gauge transformations. This, however, is not consistent for two reasons. First, since $n(\hat{x})$ depends on position, $[\hat{H}, \hat{p}_n]$ is nonzero, so that the free-particle Hamiltonian is not gauge invariant. Second, the operator $\hat{p}_n$ is not hermitian making finite gauge transformations non-unitary.

The first problem can be resolved via an abelian conversion method performed immediately at the quantum level [13]. Here one uses *operator* versions of second-class constraints $\hat{\varphi}_1 = F(\hat{x})$ and $\hat{\varphi}_2 = \hat{p}_n$ to restrict the motion to a manifold specified by $F(x) = 0$, the forbidden direction being specified by the normal vector $n(x) = \partial F(x)/|\partial F(x)|$. Then one extends the system by two extra canonical operators $\hat{Q}$ and $\hat{P}$ obeying standard Heisenberg commutation relation, and commuting with $\hat{x}$ and $\hat{p}$. The conversion of the second-class constraint operators $\hat{\varphi}_a$ is enforced by solving equations (13) and (14) with Poisson brackets replaced by commutators. The

abelian gauge generators have the same basic structure as those in (15), only that the $\hat{x}$-dependent factor of $\hat{Q}$ in $\hat{\sigma}_2$ depends now on $F(\hat{x})$. This construction solves the first problem of finding a gauge invariant Hamiltonian operator.

The hermiticity problem for the generator $\hat{\sigma}_2$ must be solved in a way that dynamics of physical degrees of freedom does not depend on the embedding procedure. For this we observe that the operator $\hat{\sigma}_2^\dagger\hat{\sigma}_2$ is just as good as $\hat{\sigma}_2$ itself to eliminate excitations of the transverse modes. It has the advantage of being hermitian. In addition, it commutes with $\hat{\sigma}_1$, so the abelian gauge algebra (13) is retained by such a choice of the second generator. Thus we modify the conversion method by taking $\hat{p}_n^\dagger\hat{p}_n$ as the constraint operator $\hat{\varphi}_2$ rather than $\hat{p}_n$. At the classical level, the new constraint $p_n^2 = 0$ is certainly equivalent to $p_n = 0$. But at the operator level, it is superior by generating unitary gauge transformations. With the new generator, the conversion equation (14) gives rise to a new Hamiltonian operator in the extended Cartesian coordinate system.

It is not hard to verify that the physical states (17) have the form $e^{iFQ/\hbar}\Psi(x)$ where $\hat{p}_n^\dagger\hat{p}_n\Psi = 0$, that is, the kinetic energy of the transverse motion is strictly zero for physical states with our choice of the gauge generators.

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